

Hexyl acetate
142-92-7 | DTXSID6022006

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 169 °C

Global applicability domain: Inside

Local applicability domain index: 1.00

Confidence level: 9.39e-01

Nearest Neighbors from the Training Set

[Image not found](#)

Methyl heptanoate

Measured: 174

Predicted: 169

[Image not found](#)

Butyl butyrate

Measured: 166

Predicted: 169

[Image not found](#)

Ethyl hexanoate

Measured: 167

Predicted: 170

[Image not found](#)

Propyl valerate

Measured: 168

Predicted: 169

[Image not found](#)

Hexyl acetate

Measured: 172

Predicted: 169